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TOWARDS A SYSTEM IN SPACE GROUP REPRESENTATIONS

V. Kopský
Institute of Physics, Czechoslovak Academy of Sciences, Na Slovance 2, P.O. Box 24, 180 40 Praha 8, Czechoslovakia

Abstract—The structure of representations of a group is tightly connected with the lattice of normal subgroups of that group. We show at first how the correlation between irreducible representations and their kernels can be used if we know the position of kernels in the lattice of normal subgroups. The rest of paper concerns the problems of deciphering the lattices of normal subgroups of space and subperiodic groups. We show that these lattices can be described easily for irreducible space groups. In case of reducible space groups we show how to get a partial description of the lattice with use of sublattices which are isomorphic images of lattices of subperiodic groups. Finally we show the ways for derivation and description of lattices of normal subgroups of subperiodic groups; in our case of layer and rod groups. Representative examples of lattices illustrate particular steps of the development of the whole scheme.

1. INTRODUCTION

The first, and so far the only one, book on four-dimensional crystallography [1] bears as its motto the famous sentence Shakespeare puts into Hamlet's mouth: "Though this be madness, yet there is method in't." As everyone, who ever tried to do a work on subgroups or on representations of three-dimensional groups, would confirm, it is not necessary to go to four dimensions; there is enough of madness in three. We are sure there is a system in it and we even know a lot about this system. Actually, we know enough to solve any particular problem of solid state physics the group theory is competent to answer. The optimism of this assertion which applies well to solution of particular cases when clever tricks and brute force might often be of help cannot be shared by those investigators who devote their efforts to global exploration of the field with aim to extract and systemize information for the benefit of more practical research. Our contemporary knowledge of the mathematics of three-dimensional symmetric systems reminds one of a big, nearly completed, jig-saw puzzle, in which some pieces are still missing and other, though properly placed, are not well orientated to meet their neighbours. It is our intention to contribute here a few new pieces to the whole picture. Our attention will be concentrated on the relationship between representations and subgroups of space and subperiodic groups. This relationship is not only one of the basic problems of structural phase transition theory but also one of the keys to systemization of representations.

2. REMEMBRANCE OF THE THINGS KNOWN

Let us first see what we have to embark from. The *International Tables for Crystallography* [2], the new edition of which recently appeared, serve traditionally as a tool for determination and description of three-dimensional periodic structures—crystals. Published by an authoritative organization, they are accepted as the world standards. There are no such recognized standards for magnetic space groups and for subperiodic groups which, up to three dimensions, are the frieze, layer and rod groups. The subperiodic groups represent, as we shall presently see, one of these jig-saw puzzle pieces which perfectly fits the picture, if we consider them in their role of factor groups of reducible space groups. It would therefore, be nice to have for them the standards which will be not only in the format of *International Tables* as Wood's tables of layer groups [3] are, but which would also be compatible with space group standards as to the orientation and choice of origin. Standards for the magnetic space groups can be obtained by a combination of *International Tables* with the tables of Shubnikov's groups [4] by setting up some correlation rules.

Representations, double-valued representations, co-representations and double-valued co-representations are as well known as the groups themselves. There are several manuals [5–7] for constructing irreducible representations or co-representations (further only ireps will be used).

Though the calculation and classification of ireps is based on the same principle of induction from ireps of translation subgroup and hence the same characteristics of ireps (**k**-vectors as points in Brillouin zone, stars, little groups and small ireps) are common to these manuals, there are at least three different arrangements of the material (by which we grouped the references), ireps are not given explicitly but need to be constructed and, last but far from least, the choice of ireps within equivalence class is not tied with any physical bases.

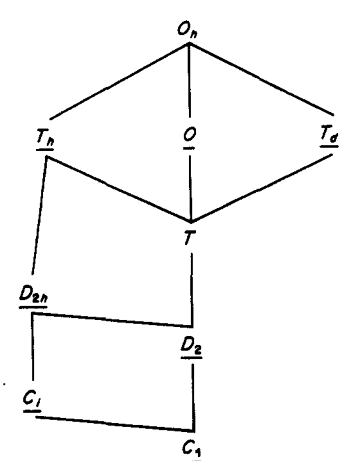
Despite these pessimistic remarks which are not meant as a criticism of the table creators, who have done a tremendous work, but as a matter-of-fact statements, the tables of ireps are a valuable part of our knowledge which proved to be useful in many applications. Together with *International Tables* they constitute a firm background for further development of group-theoretical informatics.

3. CORRELATION OF REPRESENTATIONS WITH SUBGROUPS

The problem of correlation of representations with subgroups is the key problem of the structural phase transition theory. It has been best formulated by Ascher and Kobayashi [8] as the direct and inverse Landau problem. Using Ascher's word "epikernel" of an irep $D^{(\alpha)}$ for a stabilizer of a vector of the carrier space for this representation, the problems read: (i) direct—which subgroups $H^{(\alpha)}$ of the group G are epikernels of its irep $D^{(\alpha)}$; (ii) inverse—given a subgroup H of G, is it an epikernel of some irep $D^{(\alpha)}$? What are the ireps of which it is an epikernel or, in the case that H itself is not an epikernel, how it can be expressed as an intersection of epikernels?

An ingenious way how to solve this problem in particular cases by "chain subduction criterion" [9] had been invented before epikernels were introduced and it has been later recognized as a method for identification of epikernels [10]. Ascher himself found another useful tool—the ker-core criterion. The most modern way to determine the epikernels now is the use of computers. Hatch and Stokes [11] have thus found the epikernels of ireps of plane and layer groups in points of special symmetry of the Brillouin zone and, as Professor Hatch kindly informed me, they are preparing analogous tables for space groups.

We want to talk here about a more modest problem—correlation of ireps with those normal subgroups which are their kernels. On the other hand, we do not propose just to list the normal subgroups, we want to reveal the lattices of normal subgroups from which the intersections and unions can be found. Let us first see what the advantages of correlation between ireps and their kernels are. Such a correlation enables us to tabulate ireps in one of the most natural ways. Indeed, what is it a representation of? It is a homomorphisms of a group onto another group; in our case on a certain matrix group. As a homomorphisms it is completely defined by its kernel, which is one of the normal subgroups, by its image, which is a faithful representation of the factor group by the kernel, and by the isomorphism of this factor group onto the image. Irreducible representations are the particular case os this scheme. Figure 1 illustrates the situation by the example of the point group O_h:



irep of O_h	Kernels	Images
D_2^+	T_h	C_2
D_1^-	O	C_2
D_2^-	T_d	C_2
D_3^+	D_{2h}	D_3
D_3^-	D_2	D_6
D_4^+, D_5^+	C_i	O
D_4^-, D_5^-	C_1	O_h

Fig. 1

The scheme on the l.h.s. of Fig. 1 is the lattice of normal subgroups of the group O_h. On the r.h.s. we list the ireps with their kernels and images. As images we list here the point groups, the faithful ireps of which are exactly the images of our ireps. To use the same scheme for ireps of space groups, we shall have to use the corresponding images—the irreducible matrix groups.

What is the advantage of presenting the whole lattice instead of the mere list of kernels? First, the lattice also provides information about those normal subgroups which are not kernels of any of the ireps. We have only one such group in our scheme—the group T. As we can see from the lattice, this subgroup is the intersection of any pair of the three subgroups—T_h, O, T_d. Accordingly, it is a kernel of a reducible representation which contains at least a pair of ireps, of which the groups T_h, O, T_d are the kernels.

This is a consequence of relationship between representations and normal subgroups which is expressed by "duality theorem" [12, 13]. The lattice provides further more important information, which concerns interaction of modes belonging to various ireps. There are three possible relations between normal subgroups from which the following conclusions hold about mode interaction:

(i) One group is a subgroup of the other one. For example, the group C_i is a subgroup of T_h. Then the mode belonging to irep associated with supergroup (here T_h) couples linearly with the polynomials in the mode belonging to the irep of the subgroup (C_i).

(ii) The union of subgroups which correspond to the two modes is neither of these two groups [otherwise we shall have case (i)] nor the full group (here O_h). As an example, we can take the subgroups C_i and D_2, the union of which is D_{2h}. Then the coupling between the modes is polynomial in components of both modes.

(iii) The union of subgroups which correspond to the two modes is the full group O_h. For example, we can take the group C_i and either of the groups O, T_d. Then the only allowed coupling of the modes is an invariant to invariant coupling.

These rules are the consequence of the representation generating theorem [14] and of the relationship between ireps of a group and of its factor group (engendered representations). If, in addition to the lattice we also know the extended integrity bases for matrix groups in question as we do in the presented case [15, 16] then we can write down the explicit form of interactions at once.

This scheme looks rather inviting, but an immediate practical question arises: Are lattices of normal subgroups of space groups intelligibly presentable? The answer to that question is "almost yes". Some space groups have even very simple lattices of normal subgroups and though it might seem rather surprising on the first sight, these are just the groups we would ordinarily consider more complicated—the square and hexagonal groups in two dimensions and the cubic groups in three dimensions. We shall soon see the reason for this phenomenon; let us say here that the price for the simplicity of the lattice of normal subgroups is hidden in high dimensions of corresponding ireps.

4. LATTICES OF NORMAL SUBGROUPS OF IRREDUCIBLE SPACE GROUPS

We say that the space group $\mathscr{G}$ is reducible/irreducible, if its point group G is Q-reducible/Q-irreducible [17]. Up to three dimensions the Q-reducibility/Q-irreducibility coincides with R-reducibility/R-irreducibility and irreducible are both groups $\not{p}1$, $\not{p}\bar{1}$ in one dimension, square and hexagonal groups in two dimensions and cubic groups in three dimensions. By Q and R we mean the field of rational and real numbers, respectively; the R-reducibility (irreducibility) is better known in physical applications as physical reducibility (irreducibility).

There are two main points which make the lattices of normal subgroups of irreducible space groups relatively simple. The first is the fact that only a finite number of nontrivial space groups appears in the lattice of normal subgroups. This is a consequence of "normality criterion" [18]. The number of normal subgroups of the type $P1$ (the trivial ones) is, of course, infinite. However, all these subgroups are of the same dimension as the full translation subgroup (we avoid the use of the word lattice for translation subgroup to prevent confusion with the word lattice for the partially ordered set) and hence all normal subgroups of irreducible space group with exception of the trivial point group C_1 are of finite index. In addition to that, the part of the lattice that consists of trivial space groups can be described by simple rules, especially if the irreducibility is also C-irreducibility (C—the field of complex numbers).

Indeed, let us see, for example, how such lattice looks for a cubic group of primitive Bravais type. We denote the full translation subgroup by $T(\mathbf{a}, \mathbf{b}, \mathbf{c}) = P$. The normal translation subgroups are those which are G-invariant, where G is the corresponding point group. It is a direct consequence of Schur's lemma, that we can only multiply the bases by a common factor to get the G-invariant subgroups. Hence the primitive translation subgroups, normal in the space group will be the groups $T(n\mathbf{a}, n\mathbf{b}, n\mathbf{c}) = P_n$. In addition to them, there will be also normal subgroups of the centred types I and F. We shall denote them by I_n, F_n, where index n indicates the greatest group P_n contained in I_n or F_n. In order that the groups P_n, I_n, F_n be subgroups of $P = P_1$, the indices n must be integers and in cases of subgroups I_n, F_n they must be also even. The lattice will be of the form shown in Fig. 2.

It consists of "diamonds" $P_n \langle (I_{2n}, F_{2n}) \rangle P_{2n}$ which form chains in which the groups of the next diamond have indices two times greater than those of the preceding one. This is a consequence of the relationship between groups of the types P, I, F. The group–subgroup relations between diamonds follow a law which is common for all C-irreducible cases and which can be described by the lattice of natural numbers with respect to divisibility. Indeed, let us consider only the subgroups of the P-type. The group P_m is a subgroup of P_n just if m is divisible by n. The lattice then looks like a net in a space of infinite dimension, where the axes correspond to primes. On each of these axes we have a discrete set of points, numbered by natural numbers—the powers of these primes. Thus, the number $n = p_1^{q_1} p_2^{q_2} \dots p_k^{q_k}$ has the coordinates $q_1, q_2, \dots, q_k$, on axes corresponding to primes $p_1, p_2, \dots, p_k$. Since this lattice appears in each of C-irreducible cases, we gave it the name—the principal N-factorization lattice. This lattice is also isomorphic with the lattice of subgroups of a free group with one generator which, in our context, is the group $\not{p}1$.

What is also nice is the fact that the latice of normal translation subgroups is the same for all space groups of the same Bravais class. More than that, the lattices for centred cases I and F can be evidently derived directly from the lattice of the case P. Unfortunately, the situation is so simple only in cases when the group G is C-irreducible. The lattices of normal translation subgroups for such irreducible space groups as plane groups of point classes 4, 3 and 6, where the action of point

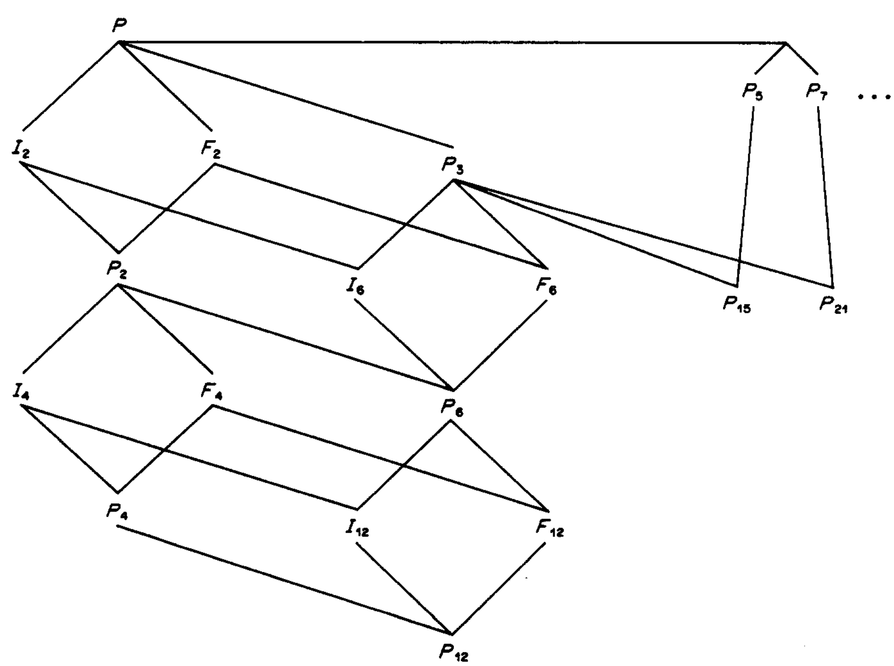


Fig. 2

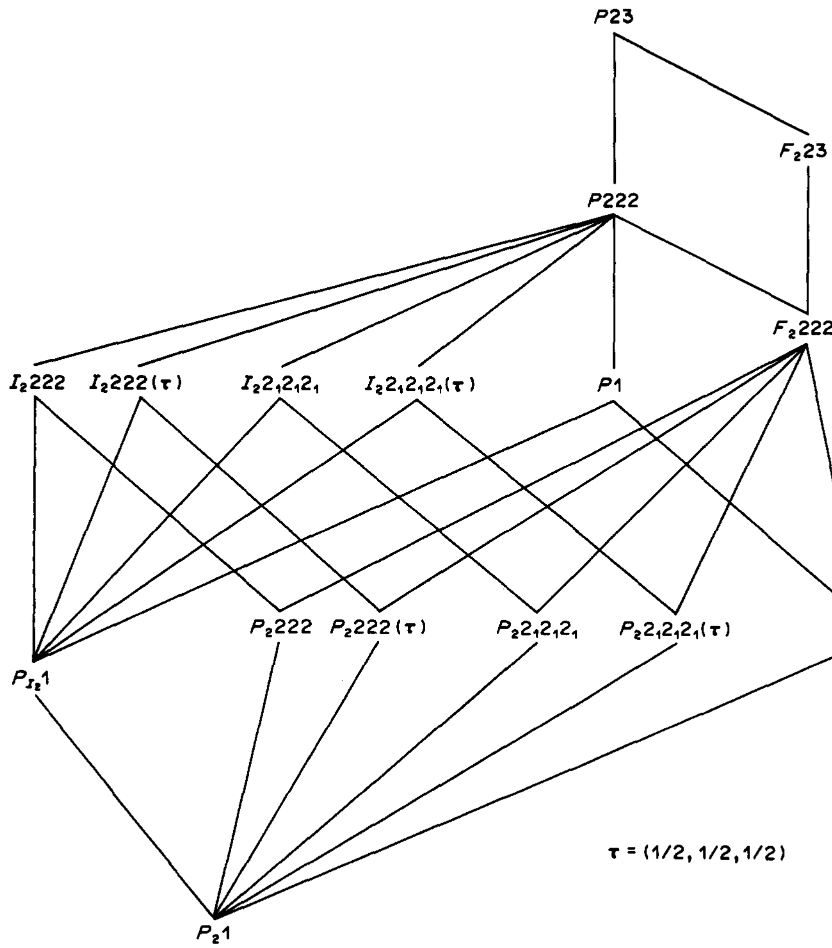


Fig. 3

group is R-irreducible but C-reducible, are more complicated, but the assertion about finite number of nontrivial normal subgroups still holds.

On the example of the lattice of normal subgroups of the space group $P23$ which is an average as complication of its structure concerns we can see how the finite bunch of nontrivial subgroups ties with the first diamond. Some notation problems need to be solved before lattices of normal subgroups can be presented for all space groups. Here we use, for example, symbols $P_{F_2}1$, $P_{I_2}1$ to denote subgroups of triclinic system and to indicate at the same time the Bravais type of the cubic system, from which they descend (see Fig. 3).

The symbol τ behind the Hermann–Mauguin symbol indicates the change of origin with respect to the standard one. A detailed global investigation of lattices of normal subgroups shows that some choices of origin and of settings (in case of orthorhombic groups), different from international standard, are preferrable.

5. REDUCIBLE SPACE GROUPS

The reducibility of a space group has several consequences which have been described by "separation diagram" and associated with it "separation theorem" [17]. One of these consequences, formulated as "factorization theorem" [19], shows that subperiodic groups appear not only as subgroups, but also as factor groups of reducible space groups. The situation is briefly described as follows: if the point group G is R-reducible (in higher dimensions Q-reducibility is required), then the vector space $V(n)$ splits under the action of G at least into two G-invariant subspaces V_1 and V_2. We shall below use the groups of tetragonal system on which the main principle may be well illustrated. These groups reduce in a unique way as also the trigonal and hexagonal groups do. Orthorhombic groups admit three reductions. In all these reductions, the subspaces V_1, V_2 are orthogonal. Monoclinic groups admit one orthogonal reduction and, together with triclinic groups, also so-called inclined reductions which need more detailed consideration.

In the following we shall use symbols $\{G, T_G, P, \mathbf{u}_G(g)\}$ for Euclidean motion groups of point class G, with G-invariant translation subgroup T_G and system of nonprimitive translations $\mathbf{u}_G$: $G \to V(n)$ with respect to the origin P. If T_G is discrete and spans the whole $V(n)$, the group is a space group in n dimensions, if T_G is discrete but spans only a subspace of $V(n)$, the group is subperiodic. Notice that in order that the group will be subperiodic, it is necessary that G be reducible.

Now we assume that the symbol denotes a space group $\mathscr{G}$, which is orthogonally reducible, so that V_1, V_2 are mutually orthogonal G-invariant subspaces. We introduce the following four groups: $T_{G1} = T_G \cap V_1$, $T_{G2} = T_G \cap V_2$; $T^0_{G1} = \sigma_1(T_G)$, and $T^0_{G2} = \sigma_2(T_G)$, where σ_1, σ_2 are projections onto spaces V_1, V_2, respectively. All four groups are G-invariant and the translation group T_G splits into:

(i) a *direct sum* $T_G = T^0_{G1} \oplus T^0_{G2} = T_{G1} \oplus T_{G2}$, if the projections are identical with intersections: $T^0_{G1} = T_{G1}$, $T^0_{G2} = T_{G2}$.

(ii) a *subdirect sum* of groups T^0_{G1}, T^0_{G2}, which is of the form:

$$T_G = T_{G1} \oplus T_{G2}[\mathbf{0} \dot{+} \mathbf{d}_2 \dot{+} \cdots \dot{+} \mathbf{d}_p],$$

where

$$T^0_{G1} = T_{G1}[\mathbf{0} \dot{+} \mathbf{d}_{21} \dot{+} \cdots \dot{+} \mathbf{d}_{p1}].$$

$$T^0_{G2} = T_{G2}[\mathbf{0} \dot{+} \mathbf{d}_{22} \dot{+} \cdots \dot{+} \mathbf{d}_{p2}].$$

Now, the groups T_{G1}, T_{G2} are G-invariant subgroups of T_G in both cases. G-invariance means that they are normal subgroups of the space group $\mathscr{G}$. The factorization theorem asserts that the factor groups $\mathscr{G}/T_{G1}$, $\mathscr{G}/T_{G2}$ are isomorphic to subperiodic groups $\mathscr{R} = \{G, T^0_{G2}, P, \mathbf{u}_{G2}(g)\}$, $\mathscr{L} = \{G, T^0_{G1}, P, \mathbf{u}_{G1}(g)\}$, respectively, where $\mathbf{u}_{G1}(g)$ are the components of the system of nonprimitive translations of $\mathscr{G}$ in V_1, V_2, respectively. Indeed, it is easy to show that Frobenius congruences for $\mathbf{u}_G(g)$ modulo T_G imply validity of Frobenius congruences of $\mathbf{u}_{G1}(g)$ modulo T^0_{G1} and of $\mathbf{u}_{G2}(g)$ modulo T^0_{G2}. Or, equivalently expressed, the factor system $\mathbf{w}_G(g, h) \in T_G$ splits into the sum of factor systems $\mathbf{w}^0_{G1}(g, h) \in T^0_{G1}$, $\mathbf{w}^0_{G2}(g, h) \in T^0_{G2}$. We denoted the factor groups by symbols $\mathscr{R}$, $\mathscr{L}$ in anticipation of three-dimensional interpretation in which the groups are the layer and rod groups.

Let us first observe that, with use of factorization, we can classify reducible space groups into layer and rod classes. The Table 1 shows the distribution of tetragonal groups with primitive Bravais type of translation subgroups.

Table 1 is, of course, formed for the space, layer and rod group types (affine classes). In rows lie the space groups of the same layer class, in columns space groups of the same rod class. The notation for layer and rod groups which lead the rows and columns is derived from notation of corresponding space groups (in a while we shall see what the word corresponding means here), in which the capital letter P is replaced by lower case p and by script $\wp$, respectively.

Table 1

C_{4v} $p4mm$ $p4bm$	$\wp 4mm$ $P4mm$ $P4bm$	$\wp 4_2cm$ $P4_2cm$ $P4_2nm$		$\wp 4cc$ $P4cc$ $P4nc$	$\wp 4_2mc$ $P4_2mc$ $P4_2bc$
D_4 $p422$ $p42_12$	$\wp 422$ $P422$ $P42_12$	$\wp 4_122$ $P4_122$ $P4_12_12$		$\wp 4_222$ $P4_222$ $P4_22_12$	$\wp 4_322$ $P4_322$ $P4_32_12$
D_{2d} $p\bar{4}2m$ $p\bar{4}2_1m$	$\wp\bar{4}2m$ $P\bar{4}2m$ $P\bar{4}2_1m$	$\wp\bar{4}2c$ $P\bar{4}2c$ $P\bar{4}2_1c$	D_{2d} $p\bar{4}m2$ $p\bar{4}b2$	$\wp\bar{4}m2$ $P\bar{4}m2$ $P\bar{4}b2$	$\wp\bar{4}c2$ $P\bar{4}c2$ $P\bar{4}n2$
D_{4h} $p4/mmm$ $p4/nbm$ $p4/mbm$ $p4/nmm$	$\wp 4/mmm$ $P4/mmm$ $P4/nbm$ $P4/mbm$ $P4/nmm$	$\wp 4/mcc$ $P4/mcc$ $P4/nnc$ $P4/mnc$ $P4/ncc$		$\wp 4_2/mmc$ $P4_2/mmc$ $P4_2/nbc$ $P4_2/mbc$ $P4_2/nmc$	$\wp 4_2/mcm$ $P4_2/mcm$ $P4_2/nnm$ $P4_2/mnm$ $P4_2/ncm$

Table 1 has a spectacular geometric interpretation in terms of space, layer and rod group diagrams. The space groups in each of the first columns have symbols identical with those of the layer groups (up to P instead of p) and their diagrams are identical with the diagrams of these layer groups. The fact that all diagrams of layer groups can be found among diagrams of space groups has been known to crystallographers for some time; we have seen the first statement of this fact in the paper by Cochran [20], who refers to a personal communication by Lonsdale. While this has not been so evident in former editions of *International Tables*, where some orthorhombic groups were given in "wrong" settings, all layer group diagrams now appear in the new edition [2], where all settings of orthorhombic groups are displayed. The diagrams of the space groups in the first rows have an analogous property; if we make a circle around origin (in some cases around another suitable point), we shall obtain a small diagram of the corresponding rod group.

Let us now look up a diagram of any group in a certain row. If we forget about components of the system of nonprimitive translations in the direction of $\mathbf{c}$ axis which means, in terms of diagram geometry, that we replace each dotted line by full one, dash-dotted by dashed, symbols of screw axes, perpendicular to the plane of the diagram, by symbols of simple axes, and if we also remove all fractions which indicate the heights of symmetry elements, parallel to the plane of diagram, which means that the elements are located now in the plane, the resulting diagram will be exactly that of the first group in the row or of the layer group, perhaps up to a shift of origin. We leave it to the reader to look up the diagrams and convince themselves how this reasoning works as well as to try and apply the same kind of reasoning to the columns, which will lead him to the diagrams of corresponding rod groups.

We shall now express these relations in an algebraic language. Let us first recall that space groups of the same arithmetic class differ by their systems of nonprimitive translations and groups, for which these systems differ only by a shift function $\varphi(g, \boldsymbol{\tau}) = \boldsymbol{\tau} - g\boldsymbol{\tau}$, belong to the same type. All these groups are extensions of translation subgroup T_G by the point group G. The space group is symmorphic, if its system of nonprimitive translations is equal just to a shift function, which means that we can make it vanish by proper choice or origin. The symmorphic group is a split extension of T_G by G or, in another terminology, a semidirect product of T_G and G. The characteristic feature of symmorphic group is the fact that it contains a group of the type G as its subgroup. The possible subgroups in this role are the site-point symmetries of certain Wyckoff positions. If the space group is not symmorphic, then none of Wyckoff positions displays the whole point symmetry G.

We can use the same language to describe the relationship of reducible space groups to layer and rod groups. Reducible space group is an extension of T^0_{G1} by $\mathscr{R}$ or of T^0_{G2} by $\mathscr{L}$. The role of the system of nonprimitive translations is now played by the components $\mathbf{u}_{G1}(g)$, $\mathbf{u}_{G2}(g)$, when T_G is the direct sum of T_{G1}, T_{G2}. The case of subdirect sum is somewhat more complicated, so let us stay with the case of direct sum to which all cases in our table belong. Space groups of the same layer class differ by the components $\mathbf{u}_{G2}(g)$ and groups for which these components differ only by shift function $\varphi(g, \boldsymbol{\tau})$ with $\boldsymbol{\tau}$ along $\mathbf{c}$ axis belong to the same type. It is therefore reasonable to use the term "symmorphic representatives of layer class" for those space groups of this class, for which $\mathbf{u}_{G2}(g)$ either vanishes or can be made to vanish by proper choice of origin, which means $\mathbf{u}_{G2}(g) = \varphi(g, \tau)$, $\boldsymbol{\tau} = a\mathbf{c}$. These symmorphic groups are then the split extensions of $T_{G2} = T^o_{G2}$ by $\mathscr{L}$ or, in other words, their semidirect products. The characteristic property of symmorphic groups of layer classes is again the fact that they contain the corresponding layer group as a subgroup. This is why the diagrams coincide—the layer group lies just in the plane of the diagram. For nonsymmorphic groups of a given layer class we shall find only fractions of the layer symmetry of this class as we follow the planes, perpendicular to c axis, along this axis. On the ground of this we have invented a procedure under the name of "scanning of layer groups" which is of interest for the theory of domain walls and twin boundaries. Quite analogously we can introduce the symmorphic representatives of rod classes and perform the scanning of rod groups—this can be actually read of directly from the diagrams of space groups.

Notice a few simple rules which hold in this scheme. For the first, each type of space group lies exactly on intersection of one layer and one rod class. The numbers of space groups are therefore the same for all layer classes as well as for all rod classes within the arithmetic class. Finally, the symmorphic space group is the symmorphic representative of both layer and rod class.

The analogy with space groups as extensions of T_G by G is, however, not complete. The algebraic reason for that lies in the fact that the point group acts on translation subgroup faithfully, which is not true as concerns the action of $\mathscr{L}$ on T^0_{G2} and of $\mathscr{R}$ on T^0_{G1}. We shall not go into the details here; they are explained in Ref. [19] for three dimensions and will be considered for arbitrary dimensions elsewhere.

6. A BRIEF REMARK ON ORIGIN CHOICES

The experience with the work on lattices of normal subgroups and on factor groups has shown us how important is a suitable system of origin choices. Indeed, if we want to specify a subgroup, we must refer to its origin with respect to the standard. The same is true for the factor groups. We have standard choice for plane and space groups in *International Tables*. There are no recognized standards for rod groups and if we want to take Wood's tables [3] of layer groups as standards, we have to take into account also a change of setting. In the table of layer and rod classes we did not bother about origins namely because of the lack of standards for layer and rod groups. We could have deduced such standard origins from the corresponding symmorphic representatives of layer and rod classes. We would have then found that it is necessary to specify shifts of origins of nonsymmorphic space groups in the table with respect to the standards in many cases.

We can do better on the ground of cohomology theory, the introduction of which to crystallography we owe to Ascher and Janner [21]. It is not necessary to go deep into this theory to understand the following argument: if we take two space groups of the same arithmetic class, then the sum of their systems of nonprimitive translations is a system of nonprimitive translations for another space group of the same arithmetic class. It is therefore natural to set up the following criterion for the choices of origins within arithmetic class: to require that the sum of the systems of nonprimitive translations of two groups, the origins of which are chosen as standard, will lead to another group, the origin of which will be also the standard one. Further: We can start from the standardization of origin choices for layer and rod groups and require that the systems of nonprimitive translations for space groups will be exactly the sums of their components for the corresponding layer and rod groups. Under these conditions we shall have no necessity for shifts of origin in our table. This is, however, not sufficient for orthorhombic groups where the settings also influence the choice.

7. LATTICES OF NORMAL SUBGROUPS OF LAYER AND ROD GROUPS AND THEIR RELATION TO LATTICES OF NORMAL SUBGROUPS OF SPACE GROUPS

The relation between point groups and equitranslational subgroups of space groups is well known. There exists a homomorphism, the kernel of which is T_G, and which maps the sublattice of equitranslational space groups onto the lattice of subgroups of the corresponding point group. The representations of point groups engender the representations of space group in Γ point of the Brillouin zone. All this is a consequence of the fact that G is isomorphic to factor group G/T_G.

Quite analogously the reducible space groups contain sublattices of those space groups which contain the partial subgroup T_{G1} or T_{G2} and which are therefore isomorphic with lattices of subgroups of corresponding rod and layer groups. The whole lattice of subgroups of a reducible space group can be then schematically presented as shown in Fig. 4.

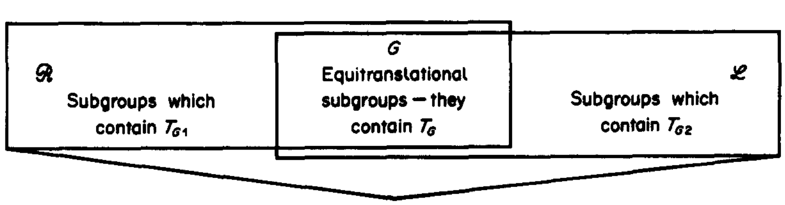


Fig. 4

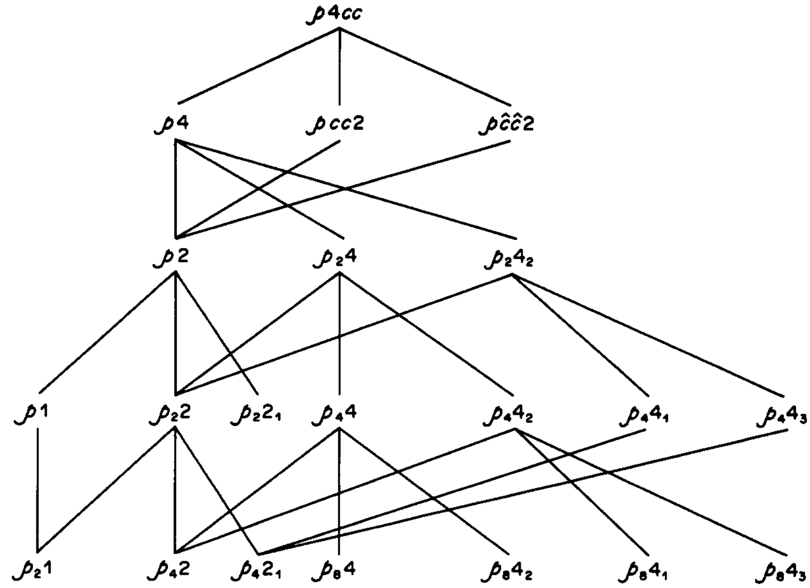


Fig. 5

The same is also true as concerns lattices of normal subgroups. To the reduction of the direct space there corresponds also the reduction of the reciprocal space and the normal subgroups in the l.h.s. sublattice will be kernels of ireps with **k**-vector on $\tilde{\mathbf{c}}$ axis, those on the r.h.s. will be kernels of ireps with **k**-vector in the $(\tilde{\mathbf{a}}, \tilde{\mathbf{b}})$-plane. Homomorphisms with kernels T_{G1}, T_{G2} map these sublattices onto the lattices of rod and layer groups and in particular they will map normal subgroups onto normal subgroups. The ireps of the rod and layer group in question will also engender ireps of the space group, the kernels of which will contain T_{G1}, T_{G2}, respectively. Let us therefore say a few words about lattices of normal subgroups of rod and layer groups.

7(a). Normal subgroups of rod groups

There exist two types of rod groups: (i) type $\not{p}H$, where the group H acts trivially on vector **c**; (ii) type $\not{p}G$, where $G = H + g_2 H$ and $g_2\mathbf{c} = -\mathbf{c}$. Groups of the type (i) contain only subgroups of the same type (i) and their nontrivial normal subgroups form infinite chains. The lattices of normal subgroups of these groups can be described by certain sublattices. Figure 5 is an example of such sublattice for the group $\not{p}4cc$.

By $\not{p}$ we denote here the translation group $T(\mathbf{c})$ and by $\not{p}_n$ the translation group $T(n\mathbf{c})$. Roofs in $\not{p}\hat{c}\hat{c}2$ indicate the pair of planes c_{xy}, $c_{x\bar{y}}$. These sublattices have to be presented up to such row from which it is clear, how the lattice structure develops to infinity. This sublattice is then repeated in the whole lattice, each time starting with the group $\not{p}_n 4cc$, where n is an even number. The connecting lines between these sublattices follow the rules of the principal N-factorization lattice from which powers of 2 are replaced by the sublattice shown above. Groups of type (i) have the property that the change of origin along **c** axis does not change them. Due to this we suggest to call them "floating groups" [more exactly, groups floating in $V(\mathbf{c})$]. In our case they, of course, coincide with "polar groups", but the term polar does not well apply when the dimension of space in which the group "flows" is higher than one. Namely the floating groups are responsible for the occurrence of infinite chains of nontrivial normal subgroups both in the lattices of subperiodic and of space groups. This assertion has a dimension independent character.

Rod groups of type (ii) contain subgroups of both types. It follows from the normality criterion that the number of normal subgroups of the type (ii) is finite. Each group of the type (ii) contains a unique equitranslational floating subgroup, so that in determining the lattice of normal subgroups of type (ii) we have to find the bunch of normal subgroups of type (ii) and to fit it with the lattice of this floating group. Let us observe, that this is a general rule, which holds actually also in the case of irreducible space groups, where the full translation subgroup plays the role of the maximal normal floating subgroup.

7(b). Normal subgroups of layer groups

In case of layer groups we have the advantage that most of them are isomorphic to plane groups. The plane groups of oblique and rectangular system are reducible and we can derive their lattices of normal subgroups from the factor groups, the role of which is taken now by frieze groups. The latter are also isomorphic to some rod groups.

The plane groups $p4$, $p4mm$, $p4gm$, $p3$, $p3m1$, $p31m$, $p6$, and $p6mm$ are irreducible; of them the groups $p4$, $p3$, $p6$ have rather complicated structure of the lattice of trivial normal subgroups because the action of the point group is C-reducible. The structure of remaining lattices of normal translation subgroups is simple; for example for the groups of square system there are two types of normal translation subgroups $-$ $p_n1 = T(n\mathbf{a}, n\mathbf{b})$ and $p_{2n}1 = T[n(\mathbf{a}+\mathbf{b}), n(\mathbf{a}-\mathbf{b})]$, the group $p_{2n}1$ is always the next subgroup to p_n1 and the structure of the lattice with respect to parameter n is that of the principal N-factorization lattice.

The layer groups are either direct or subdirect products of plane groups with the group $\{e, m_z\} = C_{sz}$. Accordingly, there exist four types of layer groups: (i) trivial layer groups—the direct products of plane groups with trivial group C_1, which differ from plane groups only by their action—we consider them as motions of three-dimensional space; (ii) groups $pG_h = pG \otimes C_{sz}$—the groups which contain explicitly reflection in the xy-plane and which are direct products; (iii) groups, in which an equitranslational halving subgroup of plane group persists unchanged, while elements of its coset are combined with reflection m_z—these have the same translation subgroup as the generating plane group; (iv) groups, in which an equiclass halving subgroup of plane group remains unchanged, while the elements of its coset are combined with reflection m_z—if the generating group is pG, then the resulting layer group is of the point class $G_h = G \otimes C_{sz}$ and its translation subgroup is a halving group of the original one. In this way we can construct all layer groups of Table 1 just from two plane groups $p4mm$ and $p4gm$. The layer groups $p4mm$, $p4bm$ are of the type (i), the groups $p4/mmm$ and $p4/mbm$ are the direct products of preceding two groups with C_{sz}, i.e. they are of the type (ii). From the group $p4mm$ we derive the groups $p422$, $p\bar{4}2m$, $p\bar{4}m2$ and from the group $p4bm$ the groups $p42_12$, $p\bar{4}2_1m$, $p\bar{4}bm$ as subdirect products of type (iii). The groups $p4/nbm$ and $p4/nmm$ are subdirect products of type (iv) derived from the group $p4mm$.

Fig. 6 represents the lattice of normal subgroups of the plane group $p4mm$ (in symbols of subgroups we use already the notation for the trivial layer groups, so that glide plane g is specified either as a or b).

Since the group $p4mm$ is irreducible, it is sufficient to attach the infinite lattice of normal translation subgroups to get the whole lattice. Due to isomorphisms, we can easily rename the groups in the lattice to get the lattices of normal subgroups of layer groups $p422$, $p\bar{4}2m$, $p\bar{4}m2$. The lattice is actually isomorphic also to the lattice of normal subgroups of groups $p4/nbm$ and $p4/nmm$ but it is more suitable to present the lattices of these groups in a somewhat different way (see below). Quite analogously Fig. 7 is isomorphic to lattices of normal subgroups of groups $p42_12$, $p\bar{4}2_1m$, and $p\bar{4}b2$. In addition to that, the lattices are homomorphic images of sublattices of space groups. Hence, when Hatch and Stokes have presented information about phase transitions in diperiodic structures, they gave actually also the same information about a whole class of phase transitions in three-dimensional structures [11].

Floating groups and hence infinite chains of normal subgroups occur also in lattices of layer groups. In oblique and rectangular case they appear already in lattices of plane groups. In square and hexagonal system they appear only for groups, the point classes of which contain explicitly the reflection m_z.

7(c). About full lattices of normal subgroups of reducible space groups

Just a few words about full lattices of normal subgroups in case of reducible space groups. There is no problem in enumeration and in finding the group–subgroup relations. The only one existing problem lies in a suitable and intelligible graphical representation. The factorization theorem is very helpful because it permits one to describe these lattices, so to say, "*per partes*". There, however, still remain two big obstacles. One of them is the presentation of lattices of normal translational

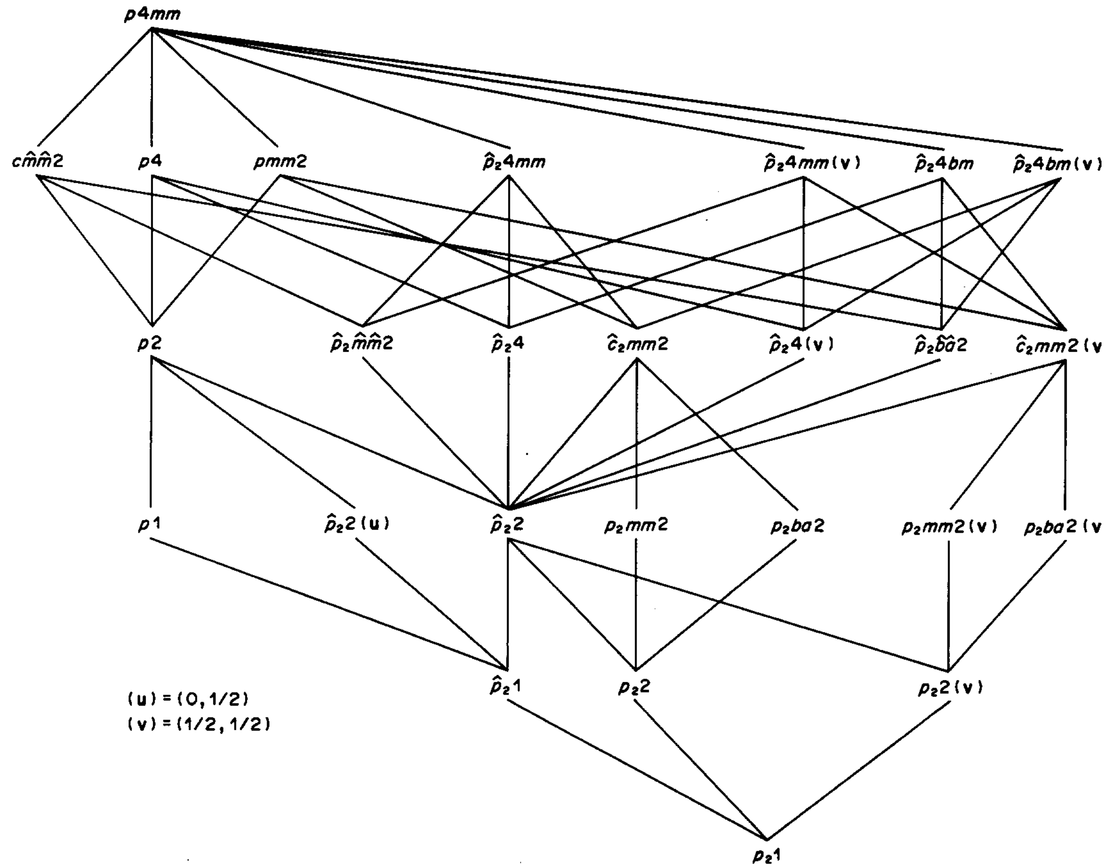

$p4mm$
$c\hat{m}\hat{m}2$
$p4$
$pmm2$
$\hat{p}_2 4mm$
$\hat{p}_2 4mm(v)$
$\hat{p}_2 4bm$
$\hat{p}_2 4bm(v)$
$p2$
$\hat{p}_2\hat{m}\hat{m}2$
$\hat{p}_2 4$
$\hat{c}_2 mm2$
$\hat{p}_2 4(v)$
$\hat{p}_2\hat{b}\hat{a}2$
$\hat{c}_2 mm2(v)$
$p1$
$\hat{p}_2 2(u)$
$\hat{p}_2 2$
$p_2 mm2$
$p_2 ba2$
$p_2 mm2(v)$
$p_2 ba2(v)$
$\hat{p}_2 1$
$p_2 2$
$p_2 2(v)$
$(u) = (0, 1/2)$
$(v) = (1/2, 1/2)$
$p_2 1$

Fig. 6

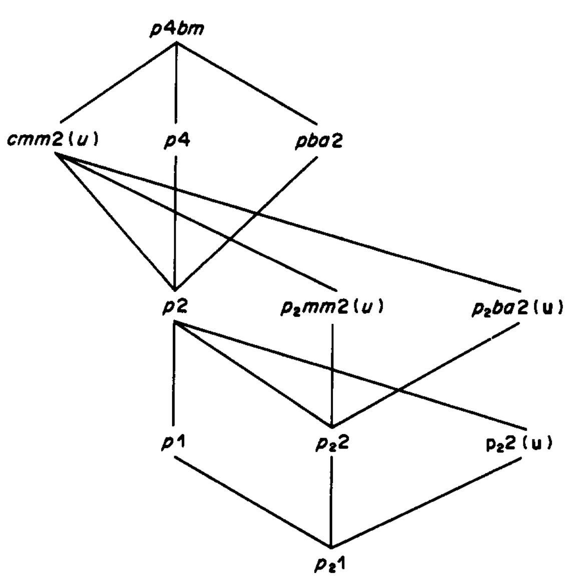

$p4bm$
$cmm2(u)$
$p4$
$pba2$
$p2$
$p_2 mm2(u)$
$p_2 ba2(u)$
$p1$
$p_2 2$
$p_2 2(u)$
$p_2 1$

Fig. 7

subgroups. Another is the big number of nontrivial normal subgroups which satisfy normality criterion. This is connected with high index of the commutator subgroup. As known, the factor group of a group by its commutator subgroup is Abelian and engenders all one-dimensional ireps. If this factor group is, for example, C_2^4, then the corresponding lattice (which appears as sublattice in our lattices) is simple to describe but rather unpleasant for graphical presentation. We have to accept it as a fact, that some of the lattices cannot be described in a compact manner.

8. VIEWS FOR THE FUTURE

We have shown here a few examples out of a work which is nearly at its end. The lattices of normal subgroups of irreducible plane and space groups and of subperiodic groups up to three dimensions have now been calculated and will be published under a special arrangement with *Czechoslovak Journal of Physics (B)*. Lattices of reducible space groups require too much volume to be published in a journal. An intelligible list of normal subgroups of space groups already exists. It has been obtained by Engel [22] with use of a computer program.

What is to be done next? The title of this contribution contains an implicite promise to introduce a system into ireps. Instead, we have dealt mainly with lattices of normal subgroups. This is not a contradiction; we believe, that namely these lattices provide one of basic keys to such system. The next thing to do is to find the correlation of normal subgroups with ireps. This includes determination of images, which are, up to now, known only for points of special symmetry of Brillouin zone. Once we know images, we can embark to such a work as determination of Clebsch–Gordan products, extended integrity bases, exomorphic types of group–subgroup relations [23], stability spaces, domain structures and decomposition of representations, induced by ireps of local symmetries. In other words, we can try to complete for space groups the same program as we have done for the point groups [12, 16, 24]. Also, we do not foresee any principal problems in extending such work eventually to magnetic space groups and co-representations.

Computers will undoubtedly play a great role in such project. Their use has been already justified [7, 11, 22]. We can anticipate their use not only for avoiding the tedious routine procedures but also for a storage of information which can be hardly published in form of tables.

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